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Dynamic modeling and optimization in membrane distillation system

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Abstract: — This paper considers a dynamic model for a direct-contact membrane distillation process based on a 2D advection-diffusion equation. Thorough analysis has been carried on the equation including descritization using an unconditionally stable algorithm with the aid of Alternating Direction Implicit method (ADI). Simulations have showed a consistency between the proposed model results and the expected behavior from the experiments. Temperature profile distribution along each membrane side, in addition to flux and flow rate variations are depicted. Distribution of temperature of all the points in feed and permeate containers has been obtained with their evolution with time. The proposed model has been validated with a data set obtained from experimental works. The comparison between the proposed model and experiments showed a matching with an error percentage less than 5%. An optimization technique was employed to find optimum values for some key parameters in the process to get certain amount of mass flux above desired values.

Keywords: Index Terms— Membrane distillation, Dynamical modeling, 2D advection diffusion, ADI discretization, Optimization.

1. INTRODUCTION

Water desalination is important to get fresh and clean water. Desalination term refers to the removal process of salt and other impurities from salty water. Moreover desalination plants turn salty water (brackish or seawater) into fresh clean water (potable or distillate water) (Close and Sorensen, 2010; Gryta, 2012). Membrane distillation (MD) is a water desalination method that can be extended to purify other solvents. It is a thermal separation process that involves transport of only water vapor or other volatile molecules through a micro porous non-wetted hydrophobic membrane. It operates on the principle of vapor-liquid equilibrium as a basis for molecular separation (Kim, 2013).

In general, feed water is heated to increase the gradient vapor pressure along the two sides of the membrane as it is the driving force, then water molecules which are adjacent to the membrane evaporate, and only vapor passes through the pores of the hydrophobic membrane to condense in the permeate side (Gryta, 2009; Lawson and Lloyd, 1997; Zhang, 2011). MD has 4 common configurations: Direct-Contact membrane distillation (DCMD), Air-Gap membrane distillation (AGMD), Vacuum membrane distillation (VMD) and Sweeping-Gas membrane distillation (SGMD). All configurations share the same principle of operation, while differ in the condensation process in the permeate side. They ensure the quality of the produced fresh water twice: firstly with the phase change from liquid to vapor, and then through the use of a membrane.

This paper considers DCMD type for modeling and discussion. Several studies have been dedicated to model DCMD (Martinez-Diez, 1999; Gryta and Tomaszewska, 1998; Khayet, 2005), they were limited to steady-state models. The need of tracking the evolution of system responses with time has been ignored. Although it is clear that the transient response for some parameters such as boundary temperature has a negligible role -since the system reaches the steady state very quickly- but we put into consideration that transient responses of temperature signal has an important role in some aspects of control, optimization and fault detection. In addition, knowing the whole response of the system helps for a better understanding of the process.

In this paper, we propose the use of an advection-diffusion equation to describe the DCMD. After start working on this model, we found that (Ashoora and Fathb, 2012) proposed the same idea without detailing the numerical implementation and the validation. Their study has not been followed by a journal paper to give all the details. We think that the analysis of the model and its validation are useful before looking at the other questions related to its control, optimization and fault detection aspects.

Through the development of the dynamic model, we propose an unconditionally stable numerical scheme to simulate the studied model, and a validation test using experimental data set that has been published in (Hwang et al., 2011). The proposed model is optimized in order to minimize the required energy, while maintaining an adequate flux throughout the operation, since DCMD suffers from energy inefficiency problems, and only small chance of energy recovery from the permeate side to the feed side (Martinez-Diez, 1999; Bui, 2007). This puts a serious drawback to its commercialization in the industry if not properly handled and optimized. Next sections present the mechanisms of heat and mass transfer in DCMD, and discuss the modeling of DCMD with advection-diffusion equation, later simulations are depicted and the process is optimized, and finally conclusions are drawn.

2. HEAT AND MASS TRANSFER MECHANISMS IN DCMD

Heat and mass transfer are coupled together in DCMD, so no heat is transferred without volatile molecules transfer. Both heat and mass are transferred from the feed side to the permeate side. Many models were proposed to describe mass and heat transfer, however they were formulated based on empirical relations and focused only on the steady-state responses of the process.

2.1 Mass transfer

Mass transfers from the feed side to the permeate side. The mechanism starts when water molecules in the feed side vaporize to be driven by vapor pressure gradient through the membrane pores, finally vapor condenses into the permeate side by the effect of the cold stream. Permeability of the membrane, and vapor pressure gradient control the mass transfer mechanism (Zhang, 2011). Mass transport mechanism in the membrane pores is directly proportional to the vapor pressure gradient through Equation (1).

$$J = C(P_1 - P_0), \tag{1}$$

where C is the membrane mass transfer coefficient of the system (Schofield, 1987). Knudsen diffusion model describes the mass transfer mechanism, this is according to the membrane pore size which is less than the mean free molecular path of the gaseous water molecules. This is the case in this paper (Schofield, 1987).

$$J_{knudsen} = 1.064 \frac{r\epsilon}{\chi^{\delta_m}} \left(\frac{M}{RT_{mean}}\right)^{0.5} (P_1 - P_0). \tag{2}$$

Table 1 illustrates the list of the used symbols.

2.2 Heat transfer

Heat transfers in membrane distillation process from the hot side to the cold side. This transfer happens across the membrane in a form of a sensible and latent heat, in addition to its transfer from the bulk flow of the feed/permeate to the boundary layer of the membrane via heat convection. Fig. 1 shows the sensible heat that is conducted from the feed side through the membrane pores to the permeate side. Whereas latent heat is carried by the water vapor. The graph shows as well the drop of the feed temperature across the boundary layer from T_f to T_1 , and the increase of the permeate temperature from T_p to T_2, this is known as the temperature polarization. The vapor pressure difference across the membrane depends on the temperature T_1 and T_2, and hereby the driving force is $P_{T_1} - P_{T_2}$ respectively.

Heat transfer was modeled previously - see (Khayet, 2005; Gryta and Tomaszewska, 1998; Martinez-Diez, 1999) -

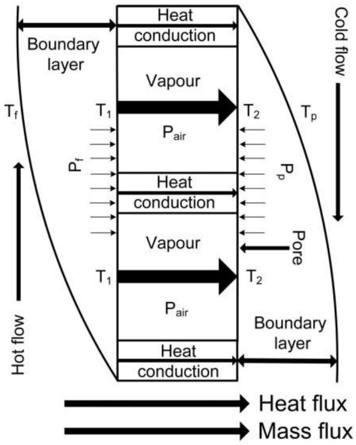

Fig. 1. DCMD heat exchange diagram. (Zhang, 2011)

through heat balance equations. Considering the energy in the process is conserved, amount of heat in feed, permeate containers as well as inside the membrane should be equal. Equations (3,4,5) show the generated amount of heat in the process.

$$Q_f = \alpha_f \, (T_f - T_1), \tag{3}$$

$$Q_p = \alpha_p \, (T_2 - T_p), \tag{4}$$

$$Q_m = \frac{k_m}{\delta_m} A(T_1 - T_2) + JH_{lat}. \tag{5}$$

2.3 Existing models

Modeling heat and mass transfer in DCMD is a hot area, and widely discussed by many researchers. (Gryta and Tomaszewska, 1998) proposed a differential equation model with respect to spatial coordinates. The model is complex and dependent on a group of semi-empirical relations gathered from experiments for membrane boundary temperatures. (Martinez-Diez and Vazquez-Gonzalez, 1999) developed an iterative method over some membrane empirical relations to reduce the error between an initial guess for the boundary layer temperatures with a pre-assumed values, they succeeded to know temperature in each experiment. (Khayet, 2005, 2011) used some empirical relations to form a simple set of equations to get the boundary layer temperatures, the equations are based on the knowledge of the heat and mass transfer coefficients, bulk fluid temperatures, and concentrations.

These models suffer from many approximation errors, since they are based on empirical relations set upon experiments. In addition, they are only valid on the adjacent layers of the membrane and provide no information for other areas in the feed or permeate containers. Moreover, they are unable to explain the behavior of the process during the transient transition, and thus cannot be relied on for detecting the occurrence of any failure.

3. ADVECTION-DIFFUSION MODEL

3.1 Introducing the model

Heat diffuses in DCMD process from the inlet of the feed stream toward the rest of the water container then exits from the bottom of the container. The diffusion of heat and its transport in the process containers is best described

Table 1. List of used symbols.

Variable	Description	Variable	Description
Q	Heat flux W	v	Flow rate m/s
T	Temperature ^oC	Cp	Specific heat $kJ/(kg.C)$
A	Membrane area m^2	ρ	Density kg/m^3
η	Gas viscosity $kg/(s.m)$	M	Molecular weight g/mol
χ	Tortuosity factor	α	Convective heat transfer coefficient $W/(m^2.K)$
J	Mass flux density $kg/(m^2.s)$	k	Thermal conductivity coefficient $W/(m.K)$
r	Membrane pore radius m	h	Heat transfer coefficient $W/(m^2.K)$
m	Membrane	Y_{ln}	Mole fraction of air
v_a	Vapor	H_{lat}	Latent heat of vaporization kJ/kg
c	Conduction	R	Gas universal constant $J/(mol.K)$
ϵ	Porosity	f	Feed
δ_m	Membrane thickness m	p	Permeate
D	Diffusion coefficient	C	Membrane mass transfer coefficient $kg/(m.hr.Pa)$

by conduction and convection mechanisms. Fig. 2 shows the basic principle of the membrane distillation process and water phase changes. The diffusion of heat inside the feed container is affected by the membrane and the permeate side as well, where two different water streams with different temperature are injected to the feed/permeate sides simultaneously. Advection-diffusion equation in two dimensions is capable of describing the heat diffusion that happens in the MD process. The interesting properties of the advection-diffusion equation made it possible to describe the convection and conduction mechanisms of the heat. The transport term in the equation represents the convection action and the conduction mechanism is represented through the second derivative term. Convection action happens along the membrane length and the conduction action happens in the direction toward and inside the membrane. Equations (6,7) illustrate the 2D advection-diffusion equation in feed and permeate sides with constant flow rates.

$$\begin{cases} \frac{\partial T_f(x,z,t)}{\partial t} + v_f \frac{\partial T_f(x,z,t)}{\partial z} = \alpha_f \frac{\partial^2 T_f(x,z,t)}{\partial x^2}, \\ 0 < x < X, 0 < z < Z,\ 0 < t < T \end{cases} \tag{6}$$

$$\begin{cases} \frac{\partial T_p(x,z,t)}{\partial t} + v_p \frac{\partial T_p(x,z,t)}{\partial z} = \alpha_p \frac{\partial^2 T_p(x,z,t)}{\partial x^2}, \\ 0 < x < X, 0 < z < Z,\ 0 < t < T \end{cases} \tag{7}$$

α_f and α_p are constants that depend on thermal conductivity (k), specific heat (cp) and the density of the seawater

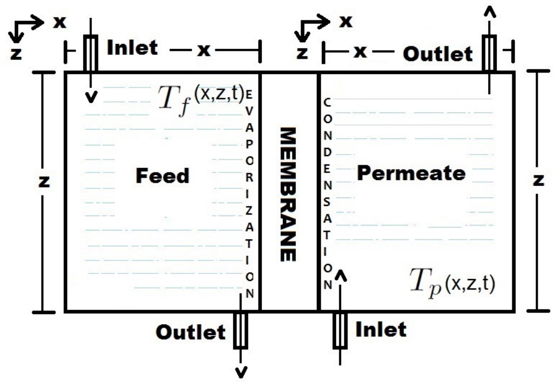

Fig. 2. Direct contact membrane distillation scheme, where it is shown the counter current injection of hot and cold streams in addition to evaporation and condensation that take place in membrane boundary layers.

(ρ) in such a formula $\alpha = \frac{k}{(cp*\rho)}$. These equations relate the temperature inside feed and permeate sides to the spatial coordinates as well as time component. Hereby, it covers heat transfer in the process and record its evolution with time. Initial profile of each water container temperature is set according to the normal operating temperatures of DCMD process:

$$T_f(x,z,0) = 60\,, T_p(x,z,0) = 20 \tag{8}$$

Boundary conditions were set based on the assumption that the process is entirely isolated from the sides of feed and permeate containers. Whereas, membrane sides are open to a heat transfer results from a mass transfer accompanies with vapor latent heat via the membrane pores as well as a temperature difference across the membrane sides. The inlets temperature of both feed and permeate sides are fixed.

$$\begin{cases} \frac{\partial T_f(0,z,t)}{\partial x} = 0, \\ \frac{\partial T_f(X)}{\partial x} = [JH_{lat} - \frac{k_m}{\delta_m}(T_f(X,z,t) - T_p(0,z,t))]/k_f, \\ T_f(x,0,t) = 60, \end{cases} \tag{9}$$

$$\begin{cases} \frac{\partial T_p(X,z,t)}{\partial x} = 0, \\ \frac{\partial T_p(X)}{\partial x} = [JH_{lat} - \frac{k_m}{\delta_m}(T_f(X,z,t) - T_p(0,z,t))]/k_p, \\ T_p(x,Z,t) = 20. \end{cases} \tag{10}$$

3.2 Numerical procedures

An approximated numerical solution is required for the 2D advection-diffusion equation, where the analytic solution is difficult to obtain. The common method for solving the heat conduction or convection equations numerically is the Crank-Nicholson method (CR), appreciating its unconditionally stability conditions. Whereas, this method results a complex set of equations in multiple dimensions, this costs too much computation effort and memory (Noye, 1989). A method called Alternating Direction Implicit method (ADI) afford a smart splitting operator that can perform the descritization with significant less computation cost using tridiagonal matrix algorithm. The idea behind the ADI is to split the finite difference equations into two simple equations. Each equation is taken implicitly with a derivative. This can be achieved by introducing an additional time n^* at the middle between time n and $n+1$ (Dehghan, 2005). Equation (11) shows the implementation with ADI.

$$\frac{u^*_{i,j}-u^n_{i,j}}{dt/2} = -a_x\frac{u^*_{i+1,j}-u^*_{i-1,j}}{2dx} + \alpha_x\frac{u^*_{i+1,j}-2u^*_{i,j}+u^*_{i-1,j}}{dx^2}$$
$$-a_z\frac{u^n_{i,j+1}-u^n_{i,j-1}}{2dz} + \alpha_z\frac{u^n_{i,j+1}-2u^n_{i,j}+u^n_{i,j-1}}{dz^2},$$

$$\frac{u^{n+1}_{i,j}-u^*_{i,j}}{dt/2} = -a_x\frac{u^*_{i+1,j}-u^*_{i-1,j}}{2dx} + \alpha_x\frac{u^*_{i+1,j}-2u^*_{i,j}+u^*_{i-1,j}}{dx^2}$$
$$-a_z\frac{u^{n+1}_{i,j+1}-u^{n+1}_{i,j-1}}{2dz} + \alpha_z\frac{u^{n+1}_{i,j+1}-2u^{n+1}_{i,j}+u^{n+1}_{i,j-1}}{dz^2}. \quad (11)$$

Fig. 3 shows the grid of descritization. It is clear how the ADI technique split the 2D PDE into 2 simple 1D ODE to be descritized . Next section deals with the simulations of the 2D advection diffusion model.

4. MODEL SIMULATION AND VALIDATION

4.1 Model simulation

The descritized model derived in the previous section is addressed twice in membrane distillation process: the first is when the evaporation takes place in the feed container, and then in the permeate container when the vapor condenses. For simulation purposes, real membrane parameters were used. The parameters values are listed in table 2. Simulations ran for 25 seconds to guarantee reaching steady-state phase. The temperature of the inlet stream in the feed side was set to 60 ^oC, however steady-state temperature was found to be less because of the effect of temperature polarization. As a result, the steady-state temperature in the permeate side was more than 20 ^0C. Fig. 4 shows the temperature profile for fixed point on membrane and variable distance toward it, the transient response lasted less than 10 seconds then all responses overlapped in the steady-state phase. This graph shows the effect of the temperature polarization on the boundary layers of the membrane. Fig. 5 depicts the temperature evolution of a fixed point on the membrane. The responses vary with time till reaching a steady-state phase. The graph shows how feed and permeate responses reached steady-state at the same time, which shows the connection between the temperature of them. It is worth mentioning that the time constant of this process is $\tau = 1.75$ seconds, and the steady-state time is $\approx 4\tau = 7$ seconds. The relation between the feed flow rate and the temperature for different flow rates is shown in Fig. 6. Feed flow rate will affect the convection heat that transferred from the feed inlet toward the container. Thus, temperature of water molecules near the inlet will increase rapidly with the flow rate. In addition, temperature polarization will increase, and the effect of the convection heat transfer will dominate the effect of the conduction heat transfer by multiple times, therefore the process will not function as needed.

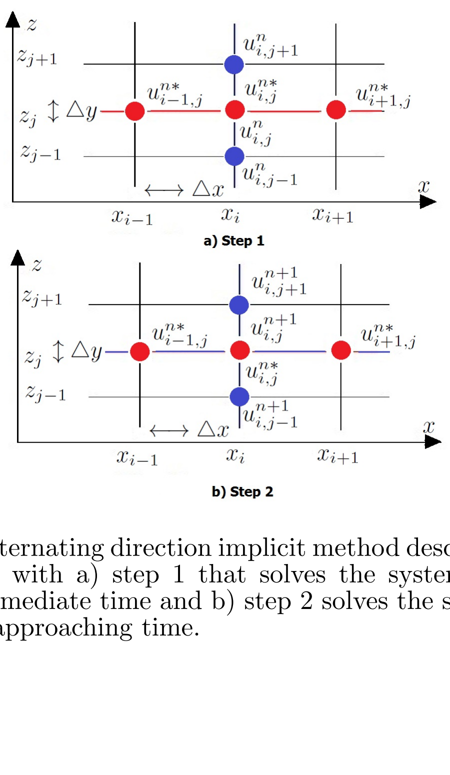

Fig. 3. Alternating direction implicit method descritization grid, with a) step 1 that solves the system for the intermediate time and b) step 2 solves the system for the approaching time.

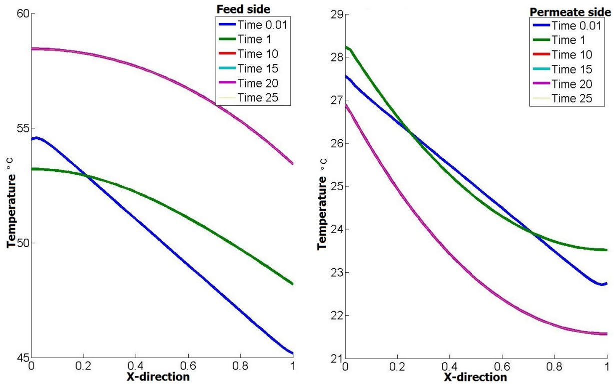

Fig. 4. Transient and steady-state response of a temperature at specific membrane module length. The responses varied with time and space evolution. At steady state responses overlapped each other like the purple response.

4.2 Model validation

The model was tested with an experimental work that has been done by (Hwang et al., 2011). In their experiments, the rate of the feed/permeate flow were equal to each other and set to multiple values. At each flow rate value, outlet temperature of the feed and the permeate were measured and recorded. Through validation process and for reliability purposes, we have set the proposed model to

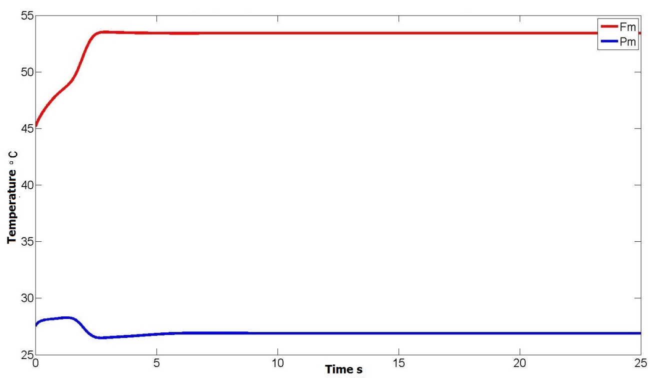

Fig. 5. Temperature evolution of a boundary layer cell with time. The red signal is for the feed response, where the blue is for the permeate response. Both responses were taken on the same membrane module length.

Table 2. Membrane distillation parameters.

Parameter	Value	Parameter	Value
Thermal conductivity constant of seawater	0.596 $W/m.K$	Seawater density	1035 kg/m^3
Thermal conductivity constant of freshwater	0.607 $W/m.K$	Freshwater density	998.2 kg/m^3
Velocity of the flow in the fresh water chamber	0.2 m/s	Membrane thickness	100μm
Average thermal conductivity of membrane and vapor	0.24 W/mK	pore size	0.3 μm
Specific heat of sea water	4180 $J/kg.C$	Porosity	75%
Velocity of the flow in the fresh water chamber	0.2 m/s	Tortuosity	1.35
Molecular weight of water	18.01489 $g/mole$		
Velocity of the flow in the seawater chamber	0.25 m/s		
Specific heat for freshwater	3850 $J/kg.C$		

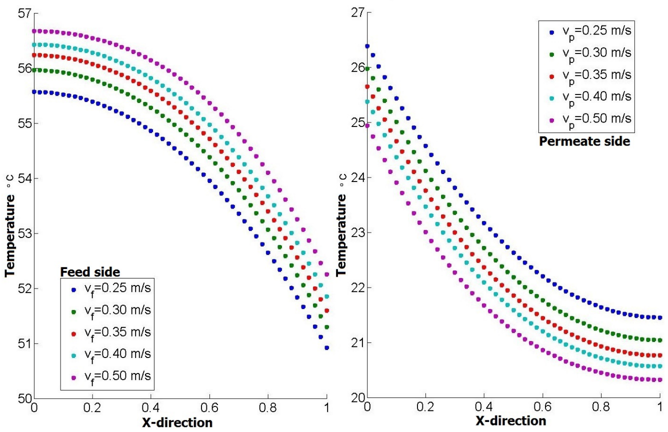

Fig. 6. The effect of the flow rate variation over the temperature distribution. It is clear how the temperature polarization coefficient increases when flow rate increases.

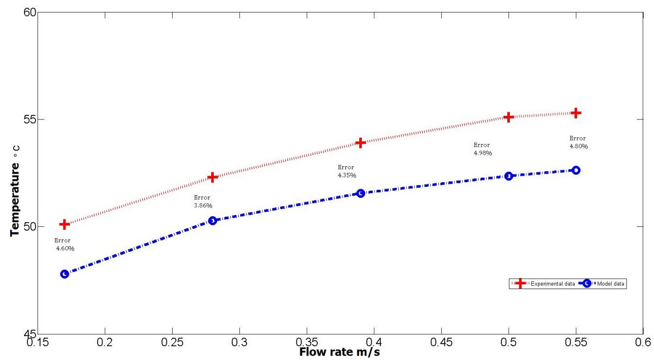

Fig. 7. Comparison between Hwang et al. experimental data set in (Hwang et al., 2011) and the 2D advection-diffusion model data. The absolute error is less than 5% between both readings.

the same membrane parameters, fluid properties and operation condition to the ones in the experiment. Comparing experiments and model data sets, the proposed model gave a close matching with an error less than 5% in the feed container to the experimental data. Fig. 7 shows the comparison between the given experimental data set and the proposed model data. The proposed model was close to the experiments when the feed flow rate was relatively high at 0.28 m/s.

5. PROCESS OPTIMIZATION

Many parameters in MD process affect the production efficiency of fresh water as well as energy consumption. As an example, thermal conductivity of the membrane impacts directly on the heat transfer, and therefore on the vapor pressure equilibrium. Most of the heat transferred across the membrane should be carried with the vapor, and heat losses due to conduction through the membrane material and convection of liquid in the boundary layers should be minimized for optimum energy efficiency (Camacho and Zhang, 2013). Parameters that affect flux are listed as the temperature difference across the membrane, the membrane support material, and thickness (Dow, 2008). The algorithm of the optimization technique is to maximize the vapor mass flux. This has to be done by increasing the temperature difference across the membrane. We performed an optimization process to set the mean vapor mass flux to be equal to 85 $g.m^{-2}hr^{-1}$ such as the cost function to be:

$$\min_{L,\delta_m,v_f,v_p} ||mean(J_{knudsen}) - 85||_2^2 \tag{12}$$

Past analysis gave a vapor mass flux mean value equal to 71.8042 $g.m^{-2}hr^{-1}$. The key parameters to be optimized are the membrane module length (L) , feed/permeate flow rate (v_f, v_p), and membrane thickness (δ_m). Table 3 shows the values of process parameters after optimization. It is an anticipated goal to have a constant temperature difference across the membrane, but it is difficult without using a controller to maintain it constant all the time.

Table 3. Optimized process parameters.

Parameter	Value
Module length (L)	0.3106 m
Membrane thickness(δ_m)	114.652 μm
Feed flow rate (v_f)	0.37496 m/s
Permeate flow rate (v_p)	0.37496 m/s

The process was optimized using Nelder-Mead technique. Optimization procedures took 48 iterations with absolute error from the desired baseline (85 $g.m^{-2}.hr^{-1}$) equal to 1.1465×10^{-4}.

Fig. 8 shows the evolution of the vapor mass flux along the optimized module length. It also shows the effect of optimization on the transferred mass flux. Optimization process can be extended to include many parameters in the DCMD operations.

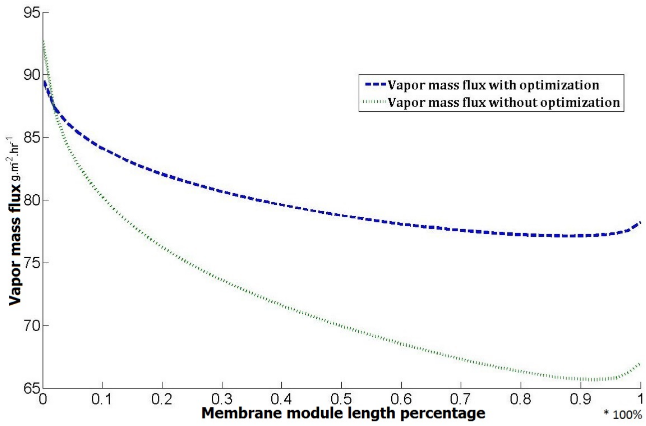

Fig. 8. A comparison between vapor mass flux before and after applying the optimization algorithm.

6. CONCLUSIONS

Understanding the mechanisms of heat transfer in DCMD is important, specially in determining the production rate of fresh water. Advection-diffusion model succeeded in relating all the mathematical parameters to physical quantities and behaviors in the process. The effect of the convection and the conduction actions were properly justified, where the process should be a trade off between the convection and conduction actions in order to have a fixed and stable production rate of fresh water. ADI method was employed in order to decrease the complexity of such systems after Crank-Nicholson descritization. The complex PDE problem was split into 2 set of 1D ODE with considering the boundary conditions. Simulations showed a matching between the derived model and the expected from literature. The presence of the time component enabled to track the response of the system even before reaching steady-state condition. Optimization techniques are important in DCMD operations, where a high constant temperature difference across the membrane has a significant role in increasing the efficiency. Optimizing key parameters in MD process leads to raise the rate of production as well as giving more stability. Membrane module length, flow rates and membrane thickness are among the important parameters to be optimized. Further work can include the modeling of membrane itself. Using mass and heat transfer techniques inside porous materials, a comprehensive temperature and heat flux distribution can be obtained. A complete model for the process then can help in manufacturing and fabricating the membrane. On the other hand, a complete model facilitates the estimation of some parameters that are difficult or expensive to be measured.

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